

Chairman's Message

CCP13 News

This has been a good year for CCP13, with an excellent annual Workshop in May, a number of visits to outstanding meetings and conferences by people sponsored by CCP13 and with many interesting publications of work in which CCP13 software has played a central part. This, our 6th CCP13 Newsletter, is the second issue of the Newsletter under its new title: "The Fibre Diffraction Review". The main credit for the very nice presentation of the "Review" should go to Geoff Mant and Richard Denny at the Daresbury Laboratory who have put in a great deal of effort to make it look good. This new edition includes many interesting articles, some arising from the May Workshop, together with Meeting/Conference reports and progress reports on new and developing CCP13 software. In addition, the Fibre Diffraction Review is being incorporated as part of the CCP13 World Wide Web pages (as with the previous Newsletters: details elsewhere).

As detailed in the report by Geoff Mant, the 1997 Annual Workshop at Daresbury was, once again, a joint meeting, with an international flavour, of CCP13 and the UK Non-Crystalline Diffraction community. This year the Meeting was somewhat experimental in format in being held over two days rather than the usual three. It was an enormous pleasure to be able to welcome to the meeting an old, and very eminent, friend, Professor Don Caspar (Florida State). He gave a splendid talk on fibre diffraction studies of Tobacco Mosaic Virus. As usual we presented prizes to the best posters as judged by Don Caspar, together with two other of our distinguished visitors from overseas, Sanjay Rastogi and Ben Hsiao.

We hope that you will come along to the 1998 Workshop (May 12-14) at Daresbury. Remember not only that your poster could win a large cash prize (1st Prize £100; 2nd Prize £50), but also that abstracts will be included in this Annual "Fibre Diffraction Review" (also on the www) - your work will be available to a worldwide audience. As usual, there will be bursaries available for students and young scientists to attend the 1998 Workshop. Details of all these are given at the end of the Newsletter.

About CCP13

CCP stands for Collaborative Computational Project. CCP13 is funded in the UK mainly by the Biotechnology and Biological Sciences Research Council (BBSRC). An additional grant comes from EPSRC to help fund meetings and travel for the "synthetic polymer" side of CCP13. CCP13 is one of 12 current CCPs run by BBSRC & EPSRC. Our current CCP runs to the end of September, 1998 with BBSRC support. The current BBSRC grant to CCP13 allows the continued employment of Richard Denny as the CCP13 RA and it provides funds towards Workshops, Newsletter Production and International Interactions. The funding by BBSRC and EPSRC also allows CCP13 to carry out "good works". Among these are schemes to fund a small number of "CCP13 Travelling Fellowships" and a "CCP13 Visiting Scientist Fellowship Program". Currently the CCP13 Committee is involved in drafting the next application to BBSRC for continued support. However, the importance of CCP13 in furthering non-crystalline diffraction applications of synchrotron radiation has been recognised by CLRC Daresbury Laboratory in that they have agreed to sponsor 50% of the Research Assistant position, currently tenanted by Richard Denny.

Your Contribution

Interested groups or individuals are invited to contact any of the officers of CCP13 to obtain information about CCP13 Workshops, software developments, software standards and so on. Offers of home-written software that could be incorporated into the new CCP13 suite of programs would be much appreciated and will, of course, permanently carry the author's attribution. Make sure that you are on the CCP13 mailing list and you will be kept informed.

Editorial Policy

Articles for inclusion in the Fibre Diffraction Review are welcome by the Editor at any time, but preferably items for the December 1998 issue should arrive before the end of November 1997. It is hoped that the Fibre Diffraction Review will become an Annual "essential" for fibre diffractionists. This is the place to advertise your fibre diffraction or NCD meetings, to report on new software or "hot" results obtained using the CCP13 or other fibre pattern processing

suites and to provide reports of meetings of interest, preferably together with one or two photographs. All technical articles will be scrutinised both for scientific content and presentational style by the Editor (or his nominee) together with at least one other member of the CCP13 Steering Panel. In this way we hope to maintain high standards. Remember that the Newsletter not only goes to other fibre diffractionists, but also to various members of the Research Council Secretariats and to other funding agencies.

International Cooperation

Although these CCPs are UK funded projects, there is a very strong interest in making them international through cooperation with interested scientists in other countries. A natural link for CCP13, for example, exists with the Special Interest Group (SIG) in Fibre Diffraction of the American Crystallographic Association and possibly with some American synchrotron users (CHESS). Others exist

with the ESRF at Grenoble and with the Photon Factory in Japan.

Retirements and New Elections

At the 1997 Annual General Meeting of CCP13, Professor Tony Ryan (Sheffield) was re-elected as a Committee member until the year 2000 and Dr. Bob Pendlebury (ICI, Wilton Centre) was elected as a replacement for Rob Rule who had resigned. This year sees the end of the periods of office of Mike Ferenczi and Trevor Forsyth. Both are prepared to stand for re-election. Other existing Committee members all continue at least until 1999. There are therefore two positions to be filled at the CCP13 Annual General Meeting in May. Any nominations for election to the Committee can be sent to the CCP13 Secretary, Dr. Geoff Mant, before the May 1998 meeting.

John Squire

IF YOU ARE A FIBRE DIFFRACTIONIST STUDYING SYNTHETIC OR BIOLOGICAL POLYMERS. THIS CCP IS FOR YOU. PLEASE HELP TO MAKE IT WORK!

International Conference on Neutron Scattering Toronto, Canada, 17-21 August 1997

This meeting attracted approximately 700 delegates from all walks of the neutron scattering world, and included sessions on biology, polymers, materials, liquids, surfaces and industrial applications. The programme was diverse and highlighted the fact that there is enormous scope for the use of neutron scattering by the CCP13/NCD community. In the Biology sessions there were presentations on computational/neutron studies of protein folding and dynamics (Jeremy Smith, Commissariat a l'Energie Atomique), quasi-Laue crystallography (Dean Myles, ILL), membrane studies (Jeremy Bradshaw, ILL), small angle neutron scattering (S. Krueger, NIST), as well a lively poster session that included presentations on actin (Ivkov, University of Maryland), DNA hydration (Shotton, Pope, Keele University), and ribosomes. In the polymer session there were talks on block copolymer phase behaviour (Bates, Minnesota), relaxation processes in glass-



forming polymers (Richter, Julich), nucleation and growth in polymer mixtures (Balsara, Polytechnic University, New York).

As with all large meetings there is often a feeling that it will be impossible to remember all of the interesting work that was presented. However, the